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Eigenvalue sensitivity to system dimensions

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ABSTRACT

Adjoint-based first-order sensitivity theory is applied to estimate the sensitivity of the k_{eff} eigenvalue to system geometric dimensions. Macroscopic cross sections in the neighborhood of a material interface are expressed in terms of a Heaviside step function. Differentiating the transport and fission operators of the transport equation with respect to the location of the interface results in a Dirac delta function. The final equation for the sensitivity has the forward-adjoint product integrals evaluated on the unperturbed interface; these are multiplied groupwise by the cross-section differences across the interface. The equation applies to the sensitivity of k_{eff} to the uniform expansion or contraction of a surface but not to a surface translation or rotation. The equation is related to an earlier one derived for internal interface perturbations in transport theory. The method is demonstrated and compared with direct perturbation calculations in spherical (r only) and cylindrical (r–z) geometries based on criticality benchmark experiments.

1. Introduction

Estimating the sensitivity of the k_{eff} eigenvalue to system parameters allows the propagation of parameter uncertainties to estimate the resulting uncertainties in k_{eff}. First-order k_{eff} sensitivity theory, based on forward and adjoint k_{eff} calculations, has been used for decades to estimate the sensitivity of k_{eff} to uncertain isotopic cross sections (Greenspan, 1976). These methods have been implemented in the widely used TSUNAMI-3D sequence (Rearden, 2006) of the SCALE code system (SCALE, 2006). However, there is also a need to estimate the sensitivity of k_{eff} to so-called non-isotopic parameters of fissionable systems (Ao, 2009; Barber and Busch, 2009), such as material dimensions, which may be uncertain due to manufacturing tolerances or imprecise or poorly documented laboratory measurements. In this paper, we apply adjoint-based first-order sensitivity theory to estimate the k_{eff} sensitivity to system dimensions.

The next section discusses transport theory and sensitivity theory and establishes notation. The derivatives of the transport operator with respect to interface locations are derived in Section 3. Section 4 discusses applications and limitations of the equations derived in Section 3. Numerical demonstrations are presented in Section 5.

2. The transport equation and sensitivity theory

The homogeneous transport equation, in multigroup form, for neutrons in a multiplying system is

$$\begin{aligned}&\widehat{\mathbf{\Omega}}\cdot\nabla\psi_0^g(r,\widehat{\mathbf{\Omega}})+\Sigma_{t,0}^g(r)\psi_0^g(r,\widehat{\mathbf{\Omega}})\\&\quad-\sum_{g'=1}^{G}\sum_{m=1}^{M}(2l_m+1)\Sigma_{sl_m,0}^{g'\to g}(r)R_m(\widehat{\mathbf{\Omega}})\varphi_{0,m}^{g'}(r)\\&=\lambda_0\sum_{g'=1}^{G}\chi_0^{g'\to g}(r)\nu\Sigma_{f,0}^{g'}(r)\varphi_{0,0}^{g'}(r),\quad g=1,\ldots,G,\end{aligned}\tag{1}$$

with the vacuum boundary condition

$$\psi_0^g(r_d,\widehat{\mathbf{\Omega}})=0,\quad \widehat{\mathbf{\Omega}}\cdot\hat{\mathbf{n}}<0,\qquad g=1,\ldots,G.\tag{2}$$

In these equations and in what follows, subscript 0 refers to the initial, unperturbed system. In addition,

$\psi^g(r,\widehat{\mathbf{\Omega}})$ angular flux of neutrons of energy group g, position r, and angle $\widehat{\mathbf{\Omega}}$
$\Sigma_t^g(r)$ total cross section at energy group g and position r
$\varphi_m^g(r)$ mth moment of the neutron angular flux at energy group g and position r
$R_m(\widehat{\mathbf{\Omega}}), l_m$ mth moment expansion function at angle $\widehat{\mathbf{\Omega}}$ and its associated coefficient
$\Sigma_{sl_m}^{g'\to g}(r)$ l_mth moment of the scattering cross section at position r from energy group g' to g and angle $\widehat{\mathbf{\Omega}}'$ to $\widehat{\mathbf{\Omega}}$
$\chi^{g'\to g}(r)$ fission spectrum at position r; neutrons born in group g due to fission induced by neutrons in group g'
$\nu\Sigma_f^g(r)$ number of neutrons per fission multiplied by fission cross section at incoming neutron group g and position r
λ eigenvalue adjusted to render the system critical
M number of expansion functions required for the particular expansion order, L (see below)
G number of energy groups
r_d and $\hat{\mathbf{n}}$ a point on the system exterior surface and the unit normal vector at that point.

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In Eq. (1), the cross section for scattering from $\hat{\Omega}'$ to $\hat{\Omega}$ has been expanded in an Lth-order Legendre polynomial of the cosine of the scattering angle, $\hat{\Omega}\cdot\hat{\Omega}'$. The addition theorem of Legendre polynomials is invoked. Each expansion function $R_m(\hat{\Omega}), m = 1,\ldots,M$ is a product of a constant, an associated Legendre polynomial, and a sine or cosine (or unity) (Alcouffe et al., 2008). M is the number of such expansion functions needed in the problem geometry for the Lth-order Legendre expansion; $m = 1$ corresponds to the zeroth moment. (In one-dimensional problems, $M = L$ and the R_m are Legendre polynomials.) The $\varphi^g_{0,m}(r)$ are the unperturbed (subscript 0) mth moments [subscript m, corresponding to expansion function $R_m(\hat{\Omega})$] of the angular flux $\psi^g_0(r,\hat{\Omega})$. The flux moments are defined in the usual way as

$$\varphi^g_m(r) \equiv \int_{4\pi} d\hat{\Omega}\, R_m(\hat{\Omega})\psi^g(r,\hat{\Omega}). \tag{3}$$

The equation adjoint to Eq. (1) is

$$\begin{aligned} &-\hat{\Omega}\cdot\nabla\psi^{*g}_0(r,\hat{\Omega}) + \Sigma^g_{t,0}(r)\psi^{*g}_0(r,\hat{\Omega}) \\ &\quad - \sum_{g'=1}^{G}\sum_{m=1}^{M}(2l_m+1)\Sigma^{g\to g'}_{sl_m,0}(r)R_m(\hat{\Omega})\varphi^{*g'}_{0,m}(r) \\ &\quad = \lambda_0 \nu\Sigma^g_{f,0}(r)\sum_{g'=1}^{G}\chi^{g\to g'}_0(r)\varphi^{*g'}_{0,0}(r), \quad g = 1,\ldots,G, \end{aligned} \tag{4}$$

with the vacuum boundary condition

$$\psi^{*g}_0(r_d,\hat{\Omega}) = 0, \hat{\Omega}\cdot\hat{\mathbf{n}} > 0, \quad g = 1,\ldots,G, \tag{5}$$

and the adjoint flux moments are defined analogously with Eq. (3) as

$$\varphi^{*g}_m(r) \equiv \int_{4\pi} d\hat{\Omega}\, R_m(\hat{\Omega})\psi^{*g}(r,\hat{\Omega}). \tag{6}$$

It can be shown (Henry, 1975) that the fundamental eigenvalues λ (or λ_0 in the specific unperturbed case) of Eqs. (1) and (4) must be equal. In normal parlance, the multiplication factor k_{eff} is defined as (Reilly et al., 1991)

$$k_{eff} \equiv \frac{1}{\lambda}. \tag{7}$$

Eqs. (1) and (4) can be rendered in operator notation as

$$(L_0 - \lambda_0 F_0)\psi_0 = 0 \tag{8}$$

and

$$(L^*_0 - \lambda_0 F^*_0)\psi^*_0 = 0, \tag{9}$$

respectively; identification of operator L and its adjoint L^* and operator F and its adjoint F^* follows immediately from comparing Eqs. (1) and (8) and Eqs. (4) and (9). The adjoint operators are defined such that

$$\langle L^*\psi^*,\psi\rangle = \langle\psi^*, L\psi\rangle \tag{10}$$

and

$$\langle F^*\psi^*,\psi\rangle = \langle\psi^*, F\psi\rangle, \tag{11}$$

where the inner product notation indicates an integral over volume and angle and a sum over energy groups.

Consider some perturbation to the system such that

$$L' = L_0 + dL, \tag{12}$$

$$F' = F_0 + dF \tag{13}$$

and

$$\lambda' = \lambda_0 + d\lambda. \tag{14}$$

In this analysis, internal operator (cross section) perturbations and internal interface (material boundary) perturbations are allowed, but boundary condition and external boundary perturbations are not. (The restriction on external boundary perturbations will be relaxed in Section 3.) The forward transport equation for the perturbed system is

$$(L' - \lambda' F')\psi' = 0, \tag{15}$$

with

$$\psi' = \psi_0 + d\psi \tag{16}$$

and the vacuum boundary condition of Eq. (2).

Multiplying Eq. (15) with the solution of Eq. (9) (the unperturbed adjoint flux) and integrating over volume and angle and summing over energy groups yields

$$\langle\psi^*_0, (L' - \lambda' F')\psi'\rangle = 0. \tag{17}$$

Using Eqs. (12)–(14) and taking advantage of Eq. (9) yields

$$\langle\psi^*_0, (dL - d\lambda F_0 - \lambda_0\, dF - d\lambda\, dF)\psi'\rangle = 0, \tag{18}$$

which can be rearranged to yield the exact equation for the eigenvalue perturbation $d\lambda$:

$$d\lambda = \frac{\langle\psi^*_0, (dL - \lambda_0\, dF)\psi'\rangle}{\langle\psi^*_0, (F_0 + dF)\psi'\rangle}. \tag{19}$$

Using Eq. (16) yields

$$d\lambda = \frac{\langle\psi^*_0, (dL - \lambda_0\, dF)\psi_0\rangle + \langle\psi^*_0, (dL - \lambda_0\, dF)d\psi\rangle}{\langle\psi^*_0, F_0\psi_0\rangle\left[1 + \dfrac{\langle\psi^*_0, dF\psi_0\rangle + \langle\psi^*_0, F_0\, d\psi\rangle + \langle\psi^*_0, dF\, d\psi\rangle}{\langle\psi^*_0, F_0\psi_0\rangle}\right]}, \tag{20}$$

still an exact expression. However, at this point terms second-order and higher in products of dL, dF, and $d\psi$ are ignored [the formula $(1+x)^{-1} = 1 - x + x^2 - \cdots$ for $|x| < 1$ is helpful here], leaving the approximation

$$d\lambda = \frac{\langle\psi^*_0, (dL - \lambda_0\, dF)\psi_0\rangle}{\langle\psi^*_0, F_0\psi_0\rangle}. \tag{21}$$

If the operators L and F depend on some set of parameters $\mathbf{u} = \{u_n, n = 1,\ldots,N\}$ and

$$\mathbf{u}' = \mathbf{u}_0 + d\mathbf{u}, \tag{22}$$

then the derivative of λ with respect to u_n is (Greenspan, 1976)

$$\frac{d\lambda}{du_n} = \frac{\left\langle\psi^*_0, \left(\frac{dL}{du_n} - \lambda_0\frac{dF}{du_n}\right)\psi_0\right\rangle}{\langle\psi^*_0, F_0\psi_0\rangle}. \tag{23}$$

From Eq. (7),

$$\frac{dk_{eff}}{d\lambda} = -\frac{1}{\lambda^2} = -k^2_{eff}, \tag{24}$$

and, using the chain rule,

$$\frac{dk_{eff}}{du_n} = -k^2_{eff,0}\frac{\left\langle\psi^*_0, \left(\frac{dL}{du_n} - \frac{1}{k_{eff,0}}\frac{dF}{du_n}\right)\psi_0\right\rangle}{\langle\psi^*_0, F_0\psi_0\rangle}. \tag{25}$$

The *sensitivity* of k_{eff} with respect to u_n is defined to be (Greenspan, 1976)

$$S_{k_{eff},u_n} \equiv \frac{u_{n,0}}{k_{eff,0}}\frac{dk_{eff}}{du_n}\bigg|_{u_n=u_{n,0}} = -k_{eff,0}u_{n,0}\frac{d\lambda}{du_n}\bigg|_{u_n=u_{n,0}}. \tag{26}$$

3. Interface shifts as operator perturbations

In this paper, we treat interface shifts as material substitutions, allowing us to write the derivatives of the L and F operators in terms of material cross sections. We use an approach very similar to that used previously (Favorite, 2004). External boundary shifts

can be accommodated merely by defining a new external boundary outside the original geometry. In this way, the original external boundary simply becomes an internal boundary, and the formalism is unchanged.

Consider the interface I_n shown in Fig. 1. Each $\hat{\mathbf{n}}$ is the outward unit normal vector at a different point on I_n. The dashed arrow represents a line $\vec{\mathbf{r}} = \vec{\mathbf{r}}_0 + r\hat{\mathbf{n}}$, where $\vec{\mathbf{r}}_0$ is a reference point anywhere along the $-\hat{\mathbf{n}}$ direction in the region below (on the negative side of) interface I_n. Let the value of the parameter $r = r_n$ define the point on I_n at which $\vec{\mathbf{r}}$ crosses I_n. The region below the interface has macroscopic cross section Σ_n and the region above (on the positive side) has cross section Σ_{n+1}. Under these conditions, in the neighborhood of the interface, along $\vec{\mathbf{r}}$, the cross section may be written

$$\Sigma(r) = \Sigma_n + H(r - r_n)(\Sigma_{n+1} - \Sigma_n), \tag{27}$$

where the Heaviside step function $H(x)$ satisfies

$$H(x) = \begin{cases} 0, & x < 0, \\ 1, & x \geqslant 0. \end{cases} \tag{28}$$

We need the cross section as a function of the interface location I_n. We imagine the point r as fixed and the point r_n as movable along $\vec{\mathbf{r}}$, use r_n as the argument of Σ in Eq. (27) (the right side is unchanged), and take the derivative of $\Sigma(r_n)$ with respect to r_n:

$$\frac{d\Sigma(r_n)}{dr_n} = -\delta(r - r_n)(\Sigma_{n+1} - \Sigma_n), \tag{29}$$

where the Dirac delta function $\delta(x)$ satisfies

$$\frac{dH(x)}{dx} = \delta(x). \tag{30}$$

We define the difference in cross sections across interface I_n as

$$\Delta\Sigma_n \equiv \Sigma_n - \Sigma_{n+1}. \tag{31}$$

Then the term in Eq. (25) involving the transport operator derivative with respect to an interface location is

$$\begin{aligned}\left\langle \psi_0^*, \frac{dL}{dr_n}\psi_0 \right\rangle = &\sum_{g=1}^{G} \int_{I_n} dS \int_{4\pi} d\hat{\mathbf{\Omega}} \psi_0^{*g}(r_n, -\hat{\mathbf{\Omega}}) \Delta\Sigma_{t,n}^{g} \psi_0^{g}(r_n, \hat{\mathbf{\Omega}}) \\ &- \sum_{g=1}^{G} \int_{I_n} dS \int_{4\pi} d\hat{\mathbf{\Omega}} \psi_0^{*g}(r_n, -\hat{\mathbf{\Omega}}) \\ &\times \sum_{g'=1}^{G} \sum_{m=1}^{M} (2l_m + 1) \Delta\Sigma_{sl_m,n}^{g' \to g} R_m(\hat{\mathbf{\Omega}}) \varphi_{0,m}^{g'}(r_n). \end{aligned} \tag{32}$$

On the right side of Eq. (32), the negative direction is used for the adjoint flux to emphasize that in the inner product, the forward and adjoint fluxes are in opposite directions. The adjoint flux moment in Eq. (4) is the usual calculational one, Eq. (6). However, it is now necessary to define an inner product adjoint flux moment as

$$\varphi_{m,IP}^{*g}(r) \equiv \int_{4\pi} d\hat{\mathbf{\Omega}} R_m(\hat{\mathbf{\Omega}}) \psi^{*g}(r, -\hat{\mathbf{\Omega}}), \tag{33}$$

where the adjoint flux is in the opposite direction of the argument of the expansion function. Eq. (32) becomes

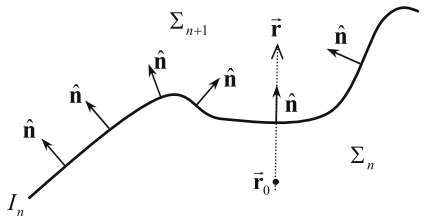

Fig. 1. Crossing an interface I_n in the outward normal direction.

$$\begin{aligned}\left\langle \psi_0^*, \frac{dL}{dr_n}\psi_0 \right\rangle = &\sum_{g=1}^{G} \sum_{m=1}^{M} (2l_m + 1) \int_{I_n} dS \Delta\Sigma_{t,n}^{g} \varphi_{0,m,IP}^{*g}(r_n) \varphi_{0,m}^{g}(r_n) \\ &- \sum_{g=1}^{G} \sum_{g'=1}^{G} \sum_{m=1}^{M} (2l_m + 1) \int_{I_n} dS \Delta\Sigma_{sl_m,n}^{g' \to g} \varphi_{0,m,IP}^{*g}(r_n) \varphi_{0,m}^{g'}(r_n). \end{aligned} \tag{34}$$

The term in Eq. (25) involving the fission operator derivative with respect to an interface location is

$$\left\langle \psi_0^*, \frac{dF}{dr_n}\psi_0 \right\rangle = \sum_{g=1}^{G} \int_{I_n} dS \int_{4\pi} d\hat{\mathbf{\Omega}} \psi_0^{*g}(r_n, -\hat{\mathbf{\Omega}}) \sum_{g'=1}^{G} \Delta\left[\chi^{g' \to g} \nu\Sigma_f^{g'}\right]_n \varphi_{0,0}^{g'}(r_n), \tag{35}$$

or, using Eq. (33),

$$\left\langle \psi_0^*, \frac{dF}{dr_n}\psi_0 \right\rangle = \sum_{g=1}^{G} \sum_{g'=1}^{G} \int_{I_n} dS \Delta[\chi^{g' \to g} \nu\Sigma_f^{g'}]_n \varphi_{0,0,IP}^{*g}(r_n) \varphi_{0,0}^{g'}(r_n). \tag{36}$$

The *IP* subscript is there for consistency; in fact $\varphi_{0,IP}^{*g}(r) = \varphi_0^{*g}(r)$, the usual adjoint scalar flux.

Using Eqs. (34) and (36), Eq. (23) (with $u_n = r_n$) becomes

$$\frac{d\lambda}{dr_n} = \frac{1}{m_f} \int_{I_n} dS \sum_{g=1}^{G} \left\{ W_g(r_n) - \sum_{g'=1}^{G} \left[W_{s,g' \to g}(r_n) + \lambda_0 W_{f,g' \to g}(r_n) \right] \right\}, \tag{37}$$

where

$$\begin{aligned} W_g(r_n) &\equiv \Delta\Sigma_{t,n}^{g} \int_{4\pi} d\hat{\mathbf{\Omega}} \psi_0^{*g}(r_n, -\hat{\mathbf{\Omega}}) \psi_0^{g}(r_n, \hat{\mathbf{\Omega}}) \\ &= \Delta\Sigma_{t,n}^{g} \sum_{m=1}^{M} (2l_m + 1) \varphi_{0,m,IP}^{*g}(r_n) \varphi_{0,m}^{g}(r_n), \end{aligned} \tag{38}$$

$$W_{s,g' \to g}(r_n) \equiv \sum_{m=1}^{M} (2l_m + 1) \Delta\Sigma_{sl_m,n}^{g' \to g} \varphi_{0,m,IP}^{*g}(r_n) \varphi_{0,m}^{g'}(r_n), \tag{39}$$

$$W_{f,g' \to g}(r_n) \equiv \Delta\left[\chi^{g' \to g} \nu\Sigma_f^{g'}\right]_n \varphi_{0,0,IP}^{*g}(r_n) \varphi_{0,0}^{g'}(r_n), \tag{40}$$

and

$$m_f \equiv \int_{dV} \sum_{g=1}^{G} \sum_{g'=1}^{G} \chi_0^{g' \to g}(r) \nu\Sigma_{f,0}^{g'}(r) \varphi_{0,0,IP}^{*g}(r) \varphi_{0,0}^{g'}(r). \tag{41}$$

The equation is written this way in order to demonstrate the correspondence with the work of Rahnema (1984), specifically his Eqs. (124)–(128). Rahnema gives the "first-order eigenvalue change due to the interior boundary (interface) perturbation" as

$$\Delta\lambda = \frac{1}{m_f} \int_{I_n} dS X_I(r_n) \sum_{g=1}^{G} \left\{ W_g(r_n) - \sum_{g'=1}^{G} \left[W_{s,g' \to g}(r_n) + \lambda_0 W_{f,g' \to g}(r_n) \right] \right\}, \tag{42}$$

where $X_I(r_n)$ is "an arbitrary first-order change in the interface points" in the direction of (or opposite) the surface normal at each point. Eq. (42) is our rendering of Rahnema's Eq. (124) using notation that has been adjusted slightly to accommodate that of this paper. Most importantly, Rahnema's $\Delta\Sigma_n$ is the opposite of ours, so there is a negative sign on the right side of his equation for $\Delta\lambda$. In addition, we have used scattering cross section and flux moments and expansions where Rahnema has retained explicit angular dependencies and integrals, and we have assumed fission neutrons are born isotropically.

The main difference between Eqs. (37) and (42) is that the former is the derivative of the λ eigenvalue with respect to the location of the interface and the latter is the eigenvalue perturbation

due to a change in the location of the interface. The function $X_I(r_n)$ is defined such that each point on the perturbed interface is obtained by displacing each point on the unperturbed interface a distance X_I in the direction of the surface normal at the point (X_I can be negative). In this context, the derivation of Eq. (37) essentially assumed that every point is displaced the *same* distance in the direction of the surface normal. The implications of this assumption are discussed in Section 4. Here, we note that if this restriction is placed on X_I in Eq. (42), then X_I is not a function of space and it can be removed from under the surface integral; Eqs. (37) and (42) are then related by

$$\Delta\lambda = \frac{d\lambda}{dr_n} X_I, \tag{43}$$

as expected.

The formalism of this section easily admits multiple interface locations for which there are known, fixed dependencies. For example, suppose the thickness of a shell is known precisely but its location is not. Let r_a, r_b, and $t = r_b - r_a$ be its inner dimension, outer dimension, and thickness, respectively. Then $d\lambda/dr_a$ and $d\lambda/dr_b$ may be computed independently, and the derivative of λ with respect to the location of the shell (inner or outer dimension) is the sum, $d\lambda/dr_a + d\lambda/dr_b$.

4. Limitations of the present derivation and implementation

The derivation of Eq. (37) in Section 3 implicitly assumes that the interface perturbation occurs such that every point on the interface is displaced the same distance in a direction parallel to the surface normal $\hat{\mathbf{n}}$ at that point (i.e., in the $+\hat{\mathbf{n}}$ or $-\hat{\mathbf{n}}$ direction). Thus, changing the *location* of an interface means, in this paper, that a curved surface is uniformly expanded or contracted with respect to its origin (which may be a line or a curve). Rotations are not allowed in this formulation, nor are translations, except for flat surfaces; for them, displacement parallel to $\hat{\mathbf{n}}$ *is* a translation of the surface.

As an example, suppose we desire to know the sensitivity of k_{eff} to the location of an absorbing sphere of fixed radius within a multiplying medium. This would be a simple translation of the sphere and Eq. (37) does not apply. However, if we desire to know the sensitivity of k_{eff} to the radius of the sphere, keeping its origin fixed, Eq. (37) can be used. In contrast, Rahnema's formula for the first-order change in the λ eigenvalue, Eq. (42), can be used for the translation of a sphere.

As another example, in a criticality experiment, a flat disk approaches another flat surface along their common axis. The flat surfaces are meant to be parallel but we do not know how parallel they are, and we desire to know the sensitivity of k_{eff} to the degree of non-parallelism – i.e., to the angle one makes with the other. This would be a rotation, and Eq. (37) does not apply. However, if we desire to know the sensitivity of k_{eff} to the distance between them, it is a translation of a flat surface and Eq. (37) can be used, but only if both sides of the moving disk are flat. In contrast, Eq. (42) can be used for a surface rotation.

For the sensitivity of k_{eff} to a surface perturbation for which Eq. (37) does not apply, a useful approach may be to use Eq. (42) with a series of perturbations $X_I^p(r_n)$, where p indicates a single value of the perturbed parameter, for example the distance of a translation or the angle of a rotation. The resulting curve of $\Delta\lambda$ vs. p can be used to find the derivative at $p = 0$.

5. Numerical demonstrations

The numerical test problems of this section used the PARTISN discrete-ordinates multigroup transport code (Alcouffe et al., 2008) for all neutron transport calculations. The convergence criterion was 10^{-6}.

Sensitivities calculated using Eq. (37) in the rightmost piece of Eq. (26) were compared with a direct perturbation method. In the direct method, interface locations were perturbed ±0.1 cm and the three points $(r_-, k_{eff}(r_-))$, $(r_0, k_{eff,0})$, and $(r_+, k_{eff}(r_+))$, where r_0 is the unperturbed interface location and $r_\pm = r_0 \pm 0.1$ cm, were fit to a line, the slope of which is the derivative dk_{eff}/du_n in Eq. (26). The minimum linear correlation coefficient C^2 [where C is Pearson's r (Press et al., 1994)] of the fit for the problems discussed below was 0.999960, indicating good (but not perfect) linearity of k_{eff} with respect to the perturbed dimensions. [When there are only three points to fit, this procedure gives the same result as fitting the points to a quadratic polynomial $k_{eff}(r) = ar^2 + br + c$ and obtaining the slope at r_0 with $dk_{eff}/dr|_{r=r_0} = 2ar_0 + b$. It also gives the same result as the central difference formula $dk_{eff}/dr|_{r=r_0} = (k_{eff}(r_+) - k_{eff}(r_-))/(r_+ - r_-)$.] The forward, adjoint, and perturbed problem inputs for each geometry all had exactly the same fine and coarse mesh structure; the geometries were perturbed by changing material assignments in coarse meshes.

In the spherical problems of Sections 5.1 and 5.3, W_g of Eq. (38) was calculated using angular fluxes [the first line in Eq. (38)]. In the cylindrical problems of Section 5.2, flux moments were used [the second line in Eq. (38)].

5.1. Godiva outer radius

A bare highly-enriched uranium (HEU) metal sphere, Godiva (LaBauve, 2002), had a radius of 8.7407 cm, a mass density of 18.74 g/cm^3, and a composition of 93.71% ^{235}U, 1.02% ^{234}U, and 5.27% ^{238}U (by weight). In this paper, transport calculations for Godiva used S_{32} quadrature, P_3 scattering, and the MENDF6 30-group cross section set (Little, 1996), which has no upscattering. The cross sections were not corrected for self-shielding. The unperturbed k_{eff} was 1.0015.

What is the total (group-summed) sensitivity of k_{eff} to the Godiva radius? The sensitivity theory value is 0.82810 and the direct perturbation value is 0.82714, a 0.1162% difference (with respect to the average). [The units of sensitivity are $\%(\Delta k_{eff}/k_{eff,0})/\%(\Delta u_n/u_{n,0})$.] These results are detailed in Table 1. This example verifies the use of the sensitivity theory approach for perturbed external problem boundaries.

5.2. Zeus fuel, moderator, and reflector dimensions

Zeus (Mosteller et al., 2004) was a cylindrical stack of alternating HEU (93% enriched) and graphite plates (the outer radius of the stack was 26.67 cm) surrounded by rectangular copper blocks. "Configuration 1" had a critical mass of 125.6 kg HEU. The two-dimensional geometry for configuration 1 as given in Appendix C of Mosteller et al. (2004) was used in this paper; in it, the rectan-

Table 1
Total sensitivity of Godiva k_{eff} to outer radius.

	Godiva outer radius
r_0, Δr (cm)	8.7407, ±0.1
$k_{eff}(r_-)$	0.99196859
$k_{eff,0}$	1.0014794
$k_{eff}(r_+)$	1.0109228
dk_{eff}/dr_n (fit)	9.477105×10^{-2}
C^2 of the fit	0.999996
Sensitivity (direct pert.)	0.82714
$d\lambda/dr_n$ [Eq. (37)]	-9.460112×10^{-2}
dk_{eff}/dr_n [Eq. (25)]	9.488123×10^{-2}
Sensitivity (sens. theory)	0.82810
Difference	0.1162%

gular copper reflector is converted to a cylindrical annulus. In this paper, transport calculations for Zeus used an S_{16} quadrature, P_3 scattering (except as noted below), and the MENDF6 30-group cross section set (Little, 1996), which has no upscattering. The cross sections were not corrected for self-shielding. The unperturbed k_{eff} was 0.9674.

What is the total (group-summed) sensitivity of k_{eff} to the radius of the HEU plates alone, to the radius of the graphite plates alone, and to the radius of the stack of HEU and graphite plates together? The sensitivity theory results are compared with the direct perturbation results in Table 2. The sensitivity theory results are in excellent agreement with the direct perturbation results, within 0.2% in all three cases. An interesting, counterintuitive result shown in Table 2 is that k_{eff} in the cylindrical Zeus is more sensitive to the radius of the graphite plates than to the radius of the HEU plates. Also note that sensitivities are additive: the k_{eff} sensitivity to the radius of the entire stack is equal to the sum of the sensitivities to the HEU and graphite plates alone.

In the cylindrical model, there is a gap of thickness 0.127 cm between the outer radius of the HEU/graphite stack and the inner radius of the copper reflector, which is 26.797 cm. What is the total (group-summed) sensitivity of k_{eff} to the inner radius of the copper reflector? The sensitivity theory value is −0.3051 and the direct perturbation value is −0.3002, a 1.62% difference (with respect to the average; this difference is discussed further below). In contrast to the results of Table 2, the negative sensitivity here means that increasing the radius decreases k_{eff}. A p% decrease in the inner radius of the copper reflector would have only a slightly smaller effect on k_{eff} than a p% increase in the HEU outer radius (from Table 2), provided that p is small enough that k_{eff} is linear.

Finally, the axial thickness of the top layer of the copper reflector is 14.4272 cm. What is the total (group-summed) sensitivity of k_{eff} to this axial thickness? In this example, the sensitivity to the thickness is obtained using the derivative of λ with respect to the location of the top reflector surface only because the bottom reflector surface is fixed. The sensitivity theory value is 0.003556 and the direct perturbation value is 0.003658, a 2.81% difference (with respect to the average; this difference is discussed further below). One might think that tightening the convergence criterion would improve the agreement, but it does not. It is no surprise that the sensitivity of k_{eff} to the thickness of the top reflector is much smaller than that to the radius of the HEU, but it is interesting to note that it is almost exactly 100 times smaller.

The results of the Zeus reflector sensitivity studies using P_3 scattering are summarized in Table 3.

A weakness of PARTISN is that the number of flux moments available in the output is limited to the number used in the expansion of the scattering source, M in Section 2. This may not be enough to accurately reconstruct the inner product involving the total cross section, W_g of Eq. (38). In other words, M may be large enough so that the scattering source is accurate, but is it large enough to guarantee that

$$\int_{4\pi} d\hat{\mathbf{\Omega}} \psi_0^{*g}(r_n, -\hat{\mathbf{\Omega}}) \Delta\Sigma_{t,n}^{g} \psi_0^{g}(r_n, \hat{\mathbf{\Omega}}) = \sum_{m=1}^{M} (2l_m + 1) \Delta\Sigma_{t,n}^{g} \varphi_{0,m,lP}^{*g}(r_n) \varphi_{0,m}^{g}(r_n) \quad (44)$$

for every group and all points on the interface I_n?

The sensitivity of the Zeus k_{eff} to the inner radius of the copper reflector and the thickness of the top copper block were recalculated using P_1 scattering in all calculations. Results are shown in Table 4. The direct perturbation sensitivities are within 1% of the results obtained when P_3 scattering was used (Table 3). The change in the adjoint-based sensitivities was 6.0% and 8.5% for the inner radius of the copper reflector and the thickness of the top copper block, respectively. The differences between the direct perturba-

Table 3
Total sensitivity of Zeus k_{eff} to reflector dimensions (P_3 scattering).

	Side reflector, inner radius	Top reflector, thickness
r_0, Δr (cm)	26.797, ±0.1	14.4272, ±0.1
$k_{eff}(r_-)$	0.96847081	0.96737318
$k_{eff,0}$	0.96739807	0.96739792
$k_{eff}(r_+)$	0.96630321	0.96742223
dk_{eff}/dr_n (fit)	-1.083800×10^{-2}	2.452500×10^{-4}
C^2 of the fit	0.999965	0.999974
Sensitivity (direct pert.)	−0.30021	0.0036575
$d\lambda/dr_n$ [Eq. (37)]	1.176963×10^{-2}	-2.547935×10^{-4}
dk_{eff}/dr_n [Eq. (25)]	-1.101471×10^{-2}	2.384507×10^{-4}
Sensitivity (sens. theory)	−0.30511	0.0035561
Difference	1.6173%	2.8114%

Table 4
Total sensitivity of Zeus k_{eff} to reflector dimensions (P_1 scattering).

	Side reflector, inner radius	Top reflector, thickness
r_0, Δr (cm)	26.797, ±0.1	14.4272, ±0.1
$k_{eff}(r_-)$	0.96675204	0.96564658
$k_{eff,0}$	0.96567159	0.96567148
$k_{eff}(r_+)$	0.96456853	0.96569584
dk_{eff}/dr_n (fit)	-1.091755×10^{-2}	2.463000×10^{-4}
C^2 of the fit	0.999964	0.999960
Sensitivity (direct pert.)	−0.30296	0.0036797
$d\lambda/dr_n$ [Eq. (37)]	1.250062×10^{-2}	-2.769152×10^{-4}
dk_{eff}/dr_n [Eq. (25)]	-1.165710×10^{-2}	2.582294×10^{-4}
Sensitivity (sens. theory)	−0.32348	0.0038580
Difference	6.5520%	4.7289%

Table 2
Total sensitivity of Zeus k_{eff} to various radii.

	HEU outer radius	Graphite outer radius	HEU + graphite outer radius
r_0, Δr (cm)	26.67, ±0.1	26.67, ±0.1	26.67, ±0.1
$k_{eff}(r_-)$	0.96613545	0.96548091	0.96422458
$k_{eff,0}$	0.96739805	0.96739805	0.96739805
$k_{eff}(r_+)$	0.96864860	0.96927697	0.97053377
dk_{eff}/dr_n (fit)	1.256575×10^{-2}	1.898030×10^{-2}	3.154595×10^{-2}
C^2 of the fit	0.999992	0.999966	0.999988
Sensitivity (direct pert.)	0.34642	0.52326	0.86968
$d\lambda/dr_n$ [Eq. (37)]	-1.345168×10^{-2}	-2.024678×10^{-2}	-3.369845×10^{-2}
dk_{eff}/dr_n [Eq. (25)]	1.258888×10^{-2}	1.894813×10^{-2}	3.153700×10^{-2}
Sensitivity (sens. theory)	0.34706	0.52238	0.86944
Difference	0.1839%	0.1696%	0.0284%

Table 5
Total sensitivity of UOFl k_{eff} to aluminum shell location.

	Shell location (inner radius)
r_0, Δr (cm)	27.9244, ±0.1
$k_{eff}(r_-)$	1.0343074
$k_{eff,0}$	1.0354058
$k_{eff}(r_+)$	1.0364955
dk_{eff}/dr_n (fit)	1.094050×10^{-2}
C^2 of the fit	0.999995
Sensitivity (direct pert.)	0.29506
$d\lambda/dr_n$ [Eq. (37)]	-1.020717×10^{-2}
dk_{eff}/dr_n [Eq. (25)]	1.094275×10^{-2}
Sensitivity (sens. theory)	0.29512
Difference	0.0206%

tion sensitivities and the adjoint-based sensitivities are 6.6% and 4.7% for the inner radius of the copper reflector and the thickness of the top copper block, respectively (Table 4), which is worse agreement than when P_3 scattering was used (Table 3). These results suggest that the ability to output more flux moments than are actually used in the transport calculation would increase the accuracy of the moments-based version of W_g of Eq. (38).

5.3. Uranium oxyfluoride solution container

A spherical highly enriched uranium oxyfluoride solution with an infinite water reflector (Pitts et al., 2004) had an outer radius of 27.9244 cm and a density of 1.0262 g/cm^3. The solution was contained in a 0.2-cm thick spherical shell of aluminum. In this paper, transport calculations for the UOFl system used S_{32} quadrature, P_3 scattering, and the BUGLE 47-group cross section set (White et al., 2000), which has thermal upscattering in four groups. The cross sections were not corrected for self-shielding. The unperturbed k_{eff} was 1.0354.

Suppose the thickness of the aluminum shell is known precisely but its location [inner radius r_a or outer radius r_b; r_a was used in Eq. (26)] is uncertain. What is the total (group-summed) sensitivity of k_{eff} to the shell inner radius? The sensitivity theory value is 0.29512 and the direct perturbation value is 0.29506, a 0.0206% difference (with respect to the average). These results are detailed in Table 5. The sensitivity theory value was obtained using the sum $d\lambda/dr_a + d\lambda/dr_b$ as discussed in Section 3.

6. Summary and conclusions

A first-order adjoint-based sensitivity-theory approach to the problem of estimating the sensitivity of k_{eff} to system dimensions (i.e., material interface locations) has been presented. Its derivation is based on representing material cross sections in the neighborhood of an interface with a Heaviside step function. The resulting equation for the derivative of the λ eigenvalue with respect to the interface location is very similar to one previously derived for the first-order estimate of the eigenvalue perturbation $\Delta\lambda$ due to an interface location perturbation (Rahnema, 1984). The main difference is that the equation in this paper only accommodates uniform expansions or contractions of a surface, while the $\Delta\lambda$ equation accommodates nonuniform surface expansions and contractions as well as rotations and translations. It should be possible to use the $\Delta\lambda$ equation to find the sensitivity of k_{eff} to surface rotations and translations. It may be possible to extend the equation of this paper to allow rotations and translations as well.

In numerical demonstrations, the method of this paper was applied to the external boundary of a one-dimensional sphere, a shell of fixed thickness in a one-dimensional sphere, and internal and external radial and axial interfaces of a two-dimensional cylinder. The sensitivity-theory approach compared very well with a direct perturbation approach. The PARTISN discrete-ordinates code was used for the neutron transport in the problems of this paper. The ability to compute and output more flux moments than are needed for the user-input scattering order in the neutron transport calculation would improve the accuracy of the sensitivity-theory results for certain cylindrical problems.

The computation of k_{eff} sensitivities to system dimensions according to the method of this paper can be incorporated into the TSUNAMI-3D framework. Forward-adjoint flux products on surfaces are required. The Monte Carlo transport code in the SCALE package, KENO (Petrie et al., 2006), does not presently have a surface flux edit (tally) capability, so that would need to be added. Care must be taken when calculating Monte Carlo surface fluxes (Favorite et al., 2009). A forward-adjoint product capability in volumes for continuous-energy k_{eff}-eigenvalue problems is under development (Kiedrowski and Brown, 2009) in the Monte Carlo code MCNP (X-5 Monte Carlo Team, 2003). If that method could be extended to compute forward-adjoint flux products on surfaces, then k_{eff} sensitivities to system dimensions may one day be computed using MCNP.

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